



chain nodes :

4 8 12 16 20 21 22 23 24 25 26 27 28 29 30 31 32 40 41 42 43 44 45

ring nodes :

1 2 3 5 6 7 9 10 11 13 14 15 17 18 19 33 34 35 36 37 38

chain bonds :

2-21 3-4 6-28 6-29 7-8 10-30 11-12 14-32 15-16 18-41 19-20 21-22 22-23 23-24
24-27 25-27 26-27 30-31 32-38 35-40 41-42 42-43 43-44 44-45

ring bonds :

1-2 1-19 2-3 3-5 5-6 6-7 7-9 9-10 10-11 11-13 13-14 14-15 15-17 17-18 18-19
33-34 33-38 34-35 35-36 36-37 37-38

exact/norm bonds :

1-2 1-19 2-3 3-4 3-5 5-6 6-7 6-28 6-29 7-8 7-9 9-10 10-11 11-12 11-13
13-14 14-15 15-16 15-17 17-18 18-19 19-20 23-24 24-27 25-27 26-27 35-40 44-45

exact bonds :

2-21 10-30 14-32 18-41 21-22 22-23 30-31 32-38 41-42 42-43 43-44

normalized bonds :

33-34 33-38 34-35 35-36 36-37 37-38

G1:H,O

Match level :

1:Atom 2:Atom 3:Atom 4:CLASS 5:Atom 6:Atom 7:Atom 8:CLASS 9:Atom 10:Atom
11:Atom 12:CLASS 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom
38:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS